

STN
registm

chain nodes :

10 11 12 19 20 21 22 23 24 25 26 27

ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17 18

chain bonds :

1-24 7-10 8-12 9-11 12-13 16-19 17-20 19-23 20-21 21-22 24-25 25-26
25-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 13-14 13-18 14-15 15-16
16-17 17-18

exact/norm bonds :

1-24 5-7 6-9 7-8 7-10 8-9 8-12 9-11 16-19 17-20 20-21 24-25 25-27

exact bonds :

12-13 19-23 21-22 25-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS11:CLASS12:CLASS13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:CLASS20:CLASS21:CLASS22:CLASS23:CLASS24:CLASS25:CLASS
26:CLASS27:CLASS

1/3

66